

Supporting Information

Water-Stable Ammonium-Terminated Carbosilane Dendrimers as Efficient Antibacterial Agents

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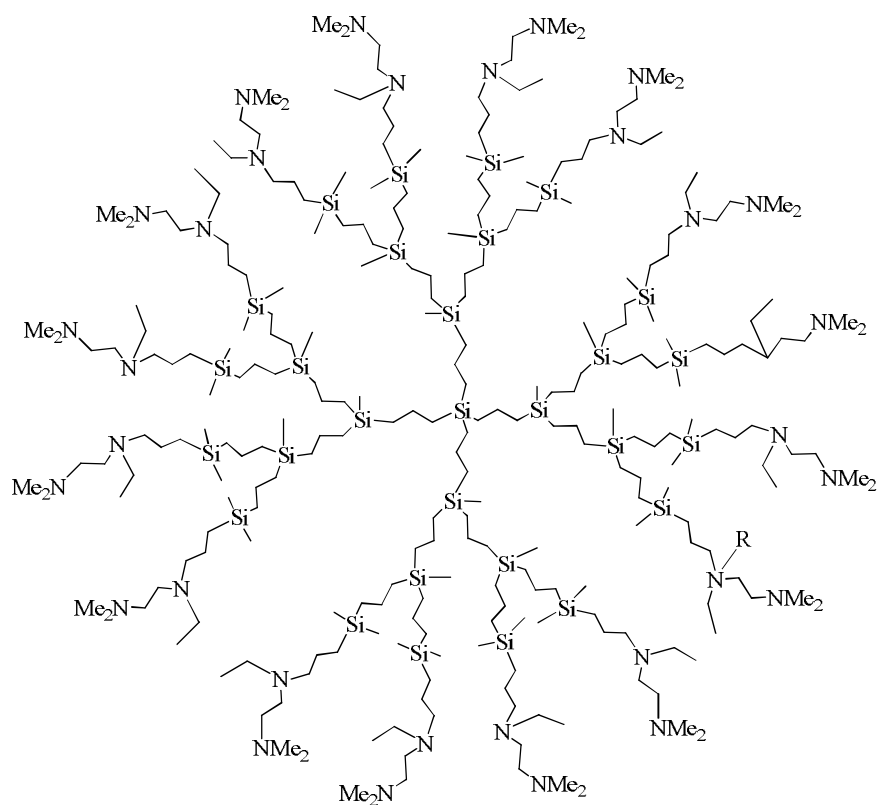
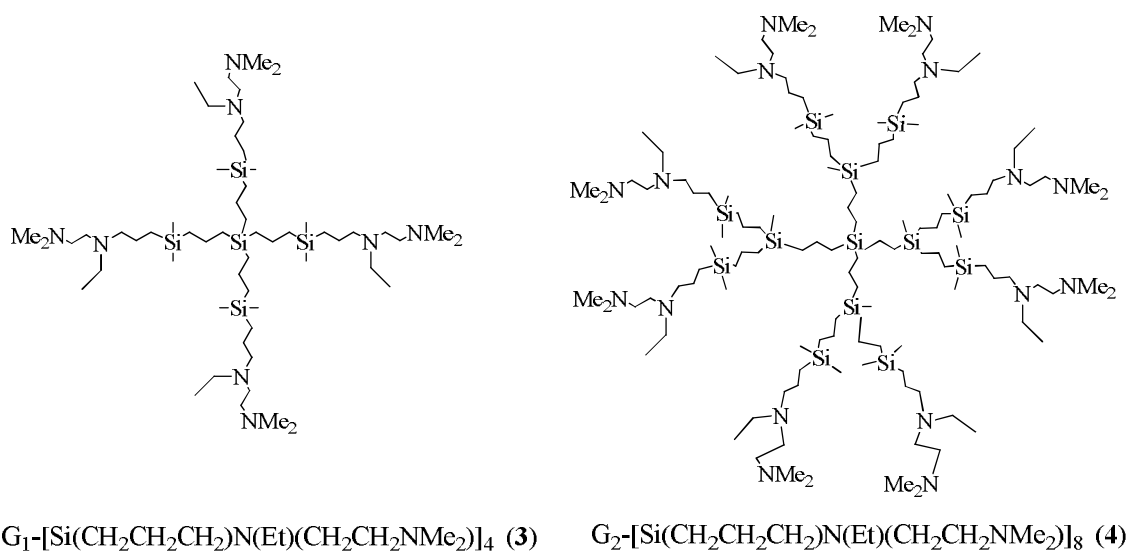


Figure S1. Molecular representation of amine-terminated carbosilane dendrimers 3-5.

A) $[(\text{CH}_2=\text{CHCH}_2)\text{N}(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}_2)]$ (1)

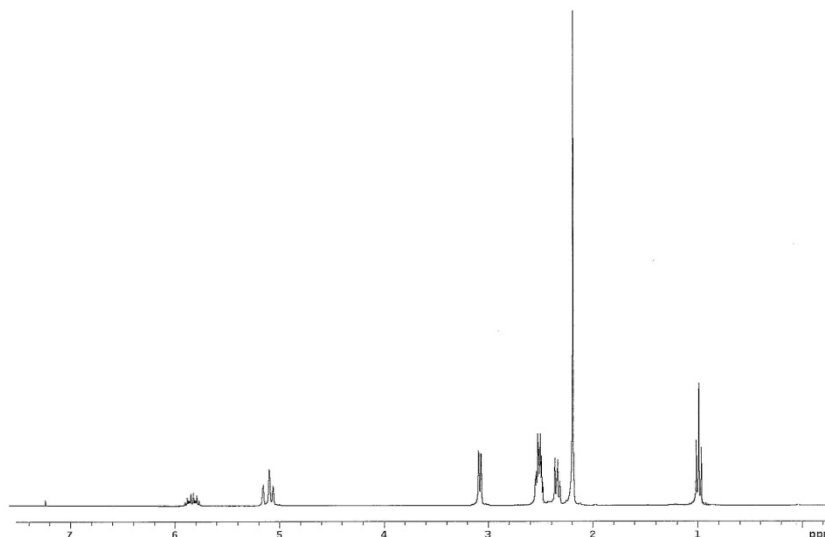


Figure S2. ^1H NMR spectrum of $[(\text{CH}_2=\text{CHCH}_2)\text{N}(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}_2)]$ (1) in CDCl_3 .

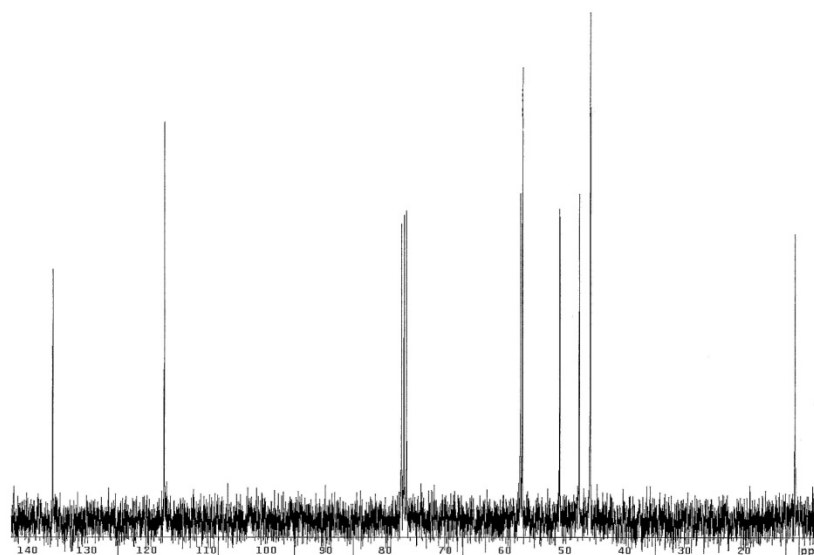


Figure S3. ^{13}C NMR spectrum of $[(\text{CH}_2=\text{CHCH}_2)\text{N}(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}_2)]$ (1) in CDCl_3 .

Adduct [(CH₂=CHCH₂)N(Et)(CH₂CH₂NMe₂)] (1)·LiBr

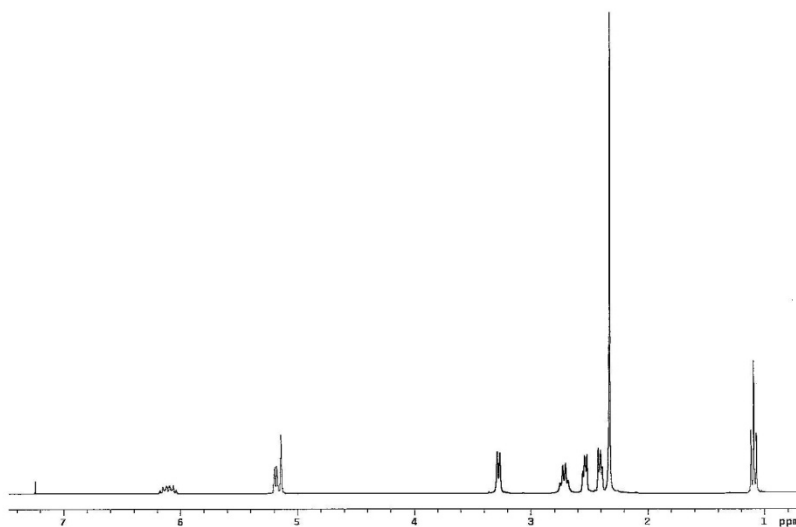


Figure S4. ¹H NMR spectrum of adduct [(CH₂=CHCH₂)N(Et)(CH₂CH₂NMe₂)] (1)·LiBr in CDCl₃.

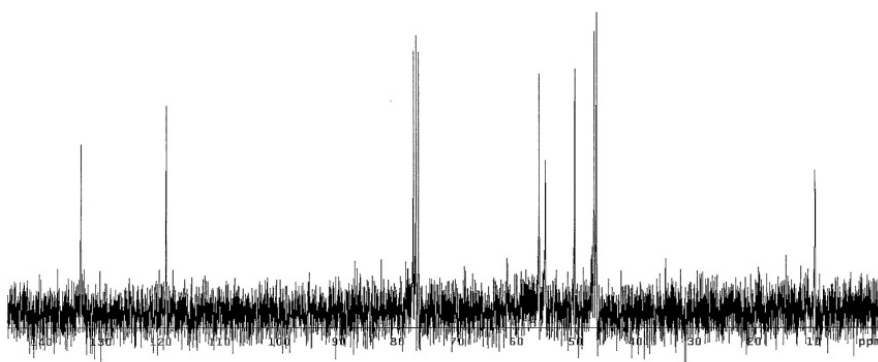


Figure S5. ¹³C NMR spectrum of adduct [(CH₂=CHCH₂)N(Et)(CH₂CH₂NMe₂)] (1)·LiBr in CDCl₃.

B) $[(Et_3SiCH_2CH_2CH_2)N(Et)(CH_2CH_2NMe_2)]$ (2)

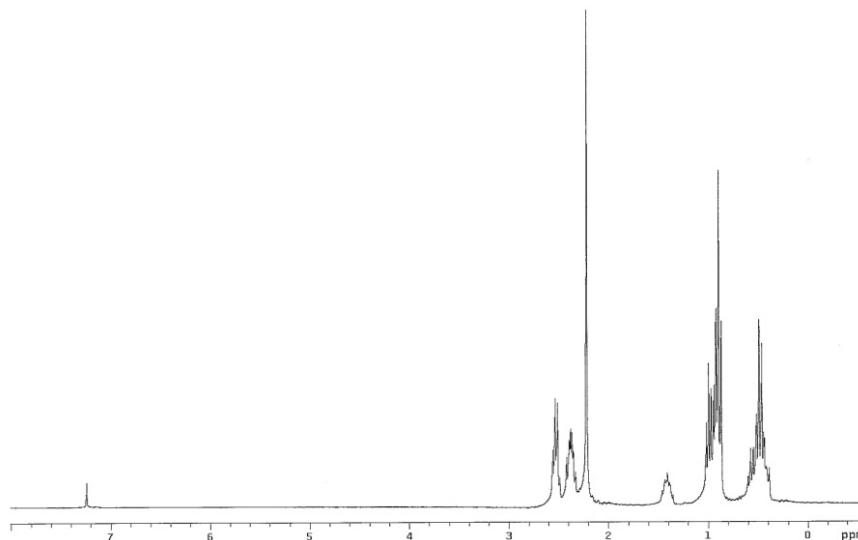


Figure S6. 1H NMR spectrum of $[(Et_3SiCH_2CH_2CH_2)N(Et)(CH_2CH_2NMe_2)]$ (2) in $CDCl_3$.

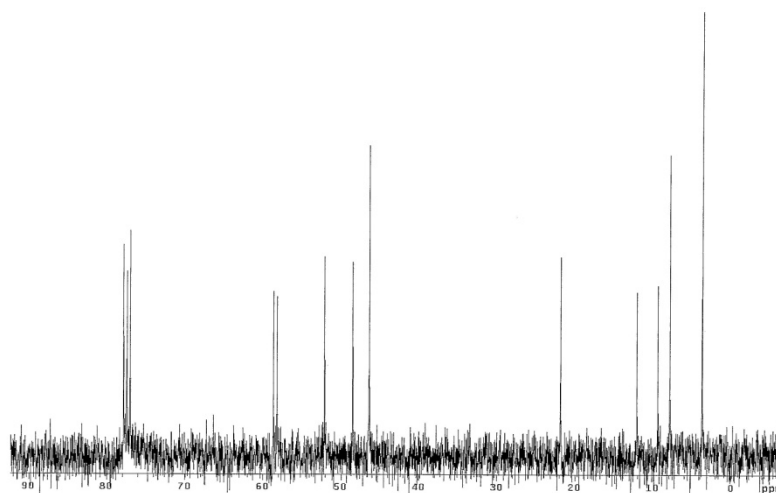


Figure S7. ^{13}C NMR spectrum of $[(Et_3SiCH_2CH_2CH_2)N(Et)(CH_2CH_2NMe_2)]$ (2) in $CDCl_3$.

C) G_1 -[Si(CH₂CH₂CH₂)N(Et)(CH₂CH₂NMe₂)]₄ (**3**)

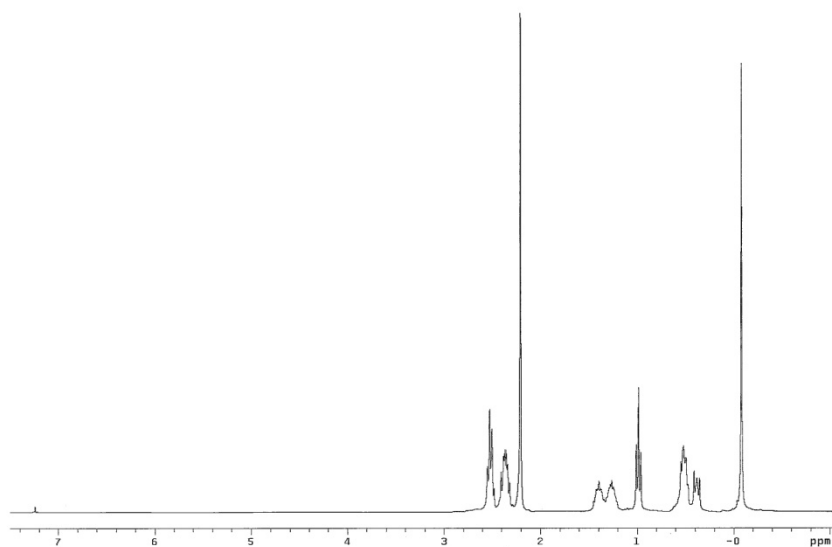


Figure S8. ¹H NMR spectrum of G_1 -[Si(CH₂CH₂CH₂)N(Et)(CH₂CH₂NMe₂)]₄ (**3**) in CDCl₃.

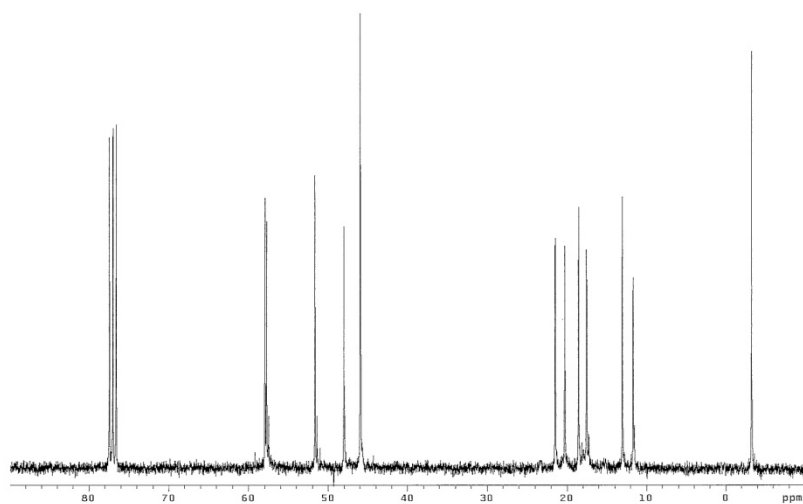


Figure S9. ¹³C NMR spectrum of G_1 -[Si(CH₂CH₂CH₂)N(Et)(CH₂CH₂NMe₂)]₄ (**3**) in CDCl₃.

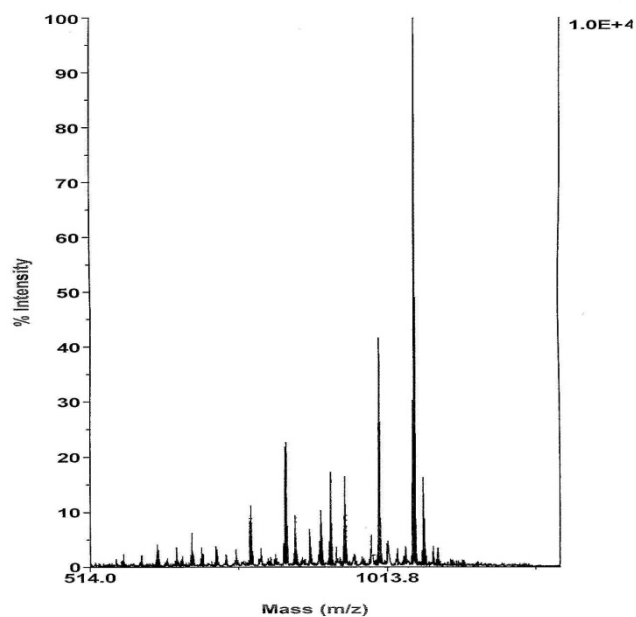


Figure S10. MALDI-TOF spectrum of G_1 -[Si(CH₂CH₂CH₂)N(Et)(CH₂CH₂NMe₂)₄ (**3**) in dithranol.

D) G_2 -[Si(CH₂CH₂CH₂)N(Et)(CH₂CH₂NMe₂)₈ (4**)**

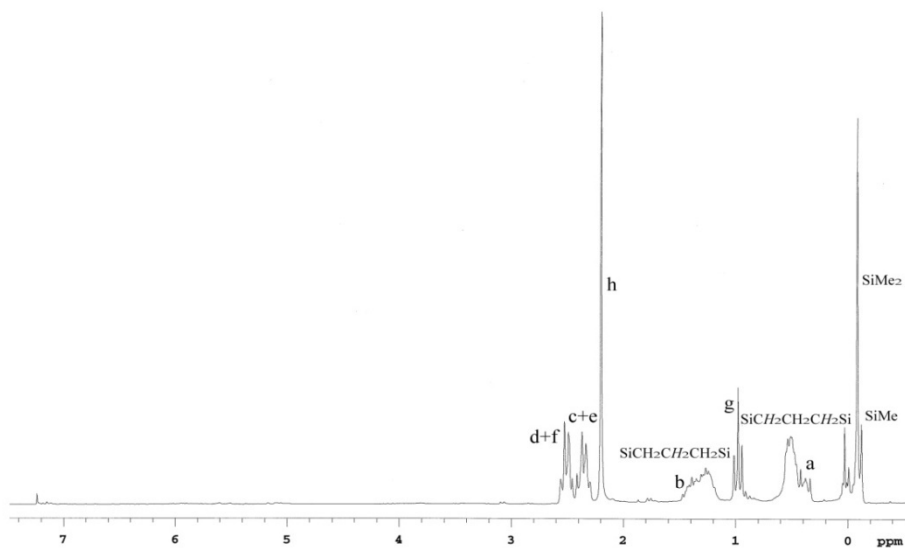


Figure S11. ¹H NMR spectrum of G_2 -[Si(CH₂CH₂CH₂)N(Et)(CH₂CH₂NMe₂)₈ (**4**) in CDCl₃.

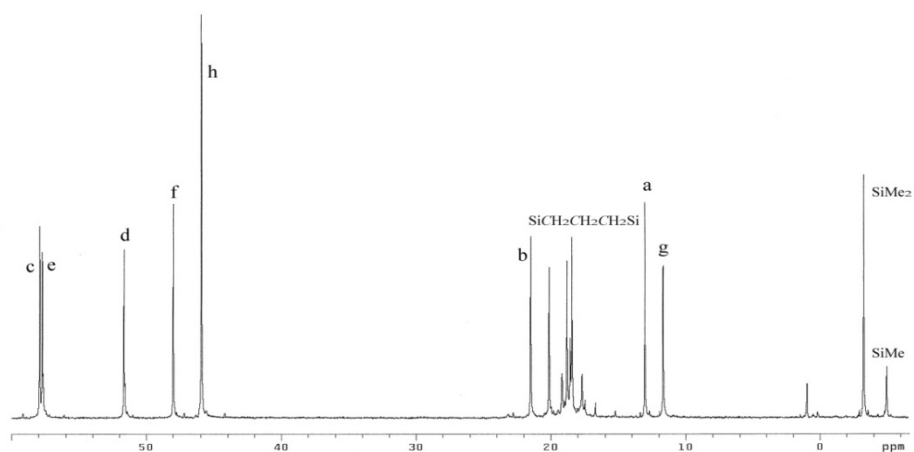


Figure S12. ^{13}C NMR spectrum of $\text{G}_2\text{-}[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}_2)]_8$ (**4**) in CDCl_3 .

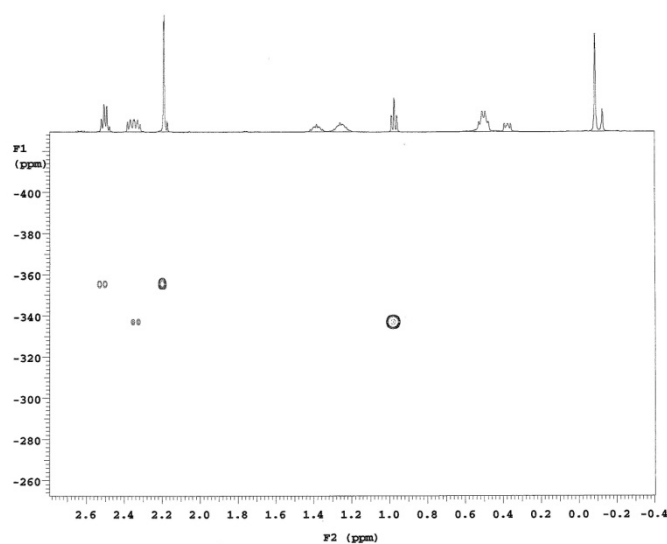


Figure S13. HMBC $\{^1\text{H}\text{-}^{15}\text{N}\}$ spectrum of $\text{G}_2\text{-}[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}_2)]_8$ (**4**) in CDCl_3 .

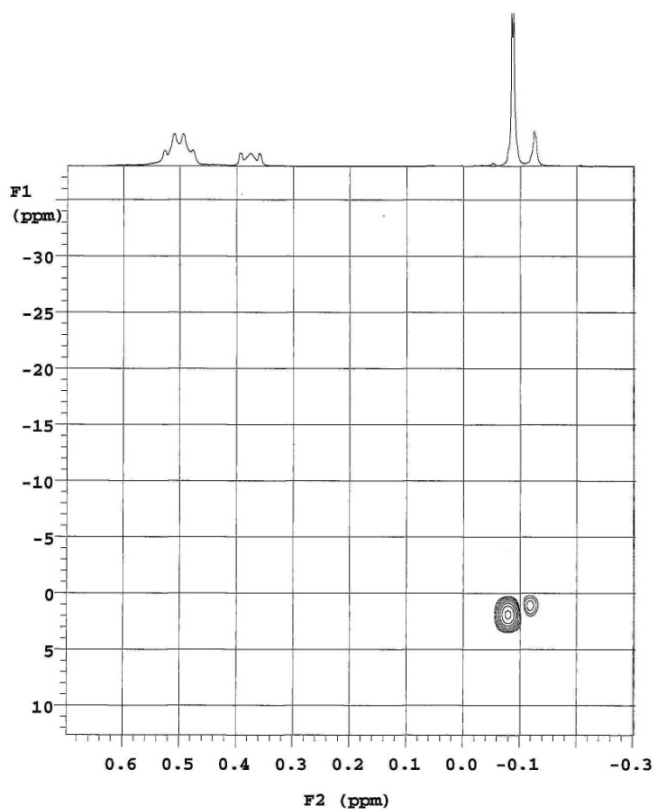


Figure S14. HMBC $\{^1\text{H}-^{29}\text{Si}\}$ spectrum of $\text{G}_2\text{-}[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}_2)]_8$ (**4**) in CDCl_3 .

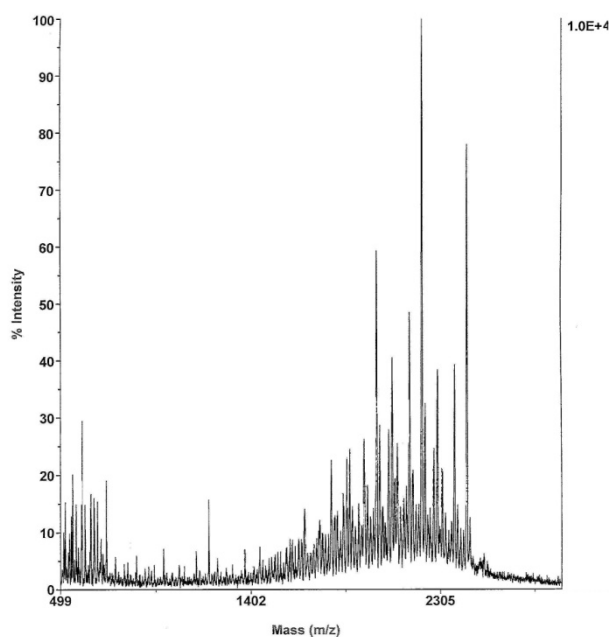


Figure S15. MALDI-TOF spectrum of $\text{G}_2\text{-}[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}_2)]_8$ (**4**) in dithranol.

E) **G₃-[Si(CH₂CH₂CH₂)N(Et)(CH₂CH₂NMe₂)]₁₆ (5)**

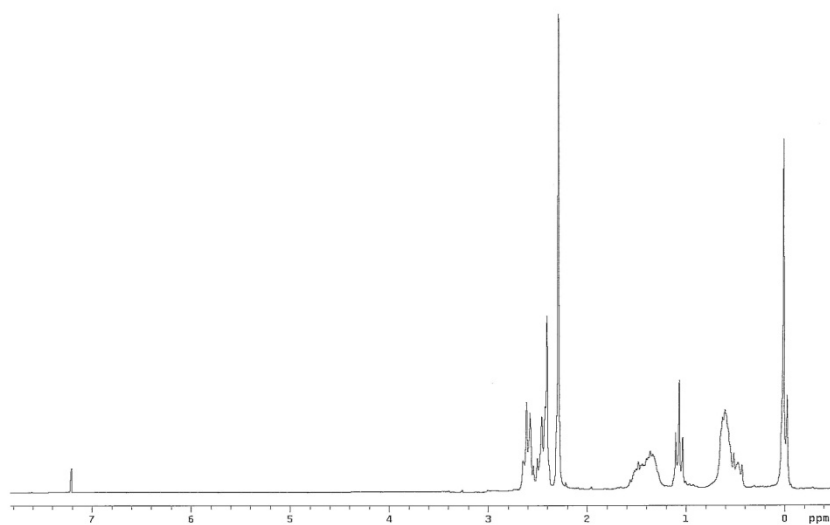


Figure S16. ¹H NMR spectrum of G₃-[Si(CH₂CH₂CH₂)N(Et)(CH₂CH₂NMe₂)]₁₆ (5) in CDCl₃.

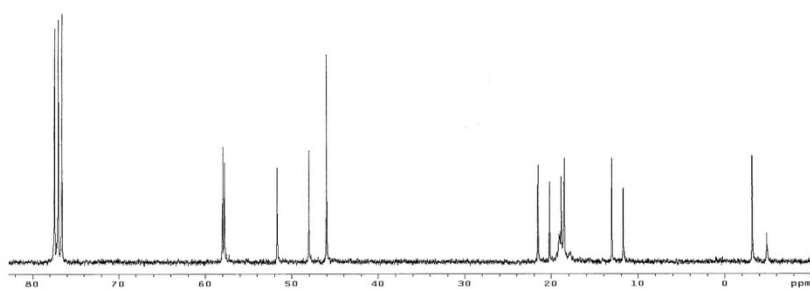


Figure S17. ¹³C NMR spectrum of G₃-[Si(CH₂CH₂CH₂)N(Et)(CH₂CH₂NMe₂)]₁₆ (5) in CDCl₃.

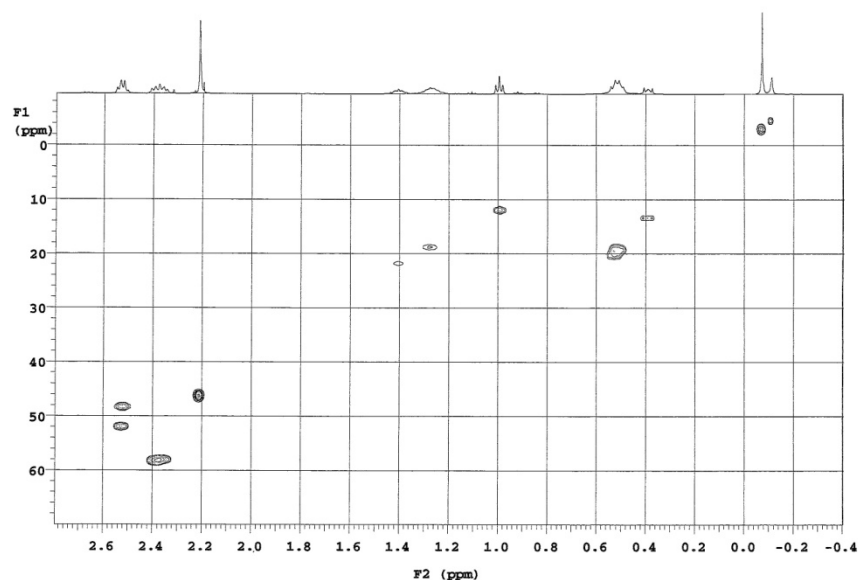


Figure S18. HMQC- $\{^1\text{H}-^{13}\text{C}\}$ spectrum of $\text{G}_3\text{-}[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}_2)]_{16}$ (**5**) in CDCl_3 .

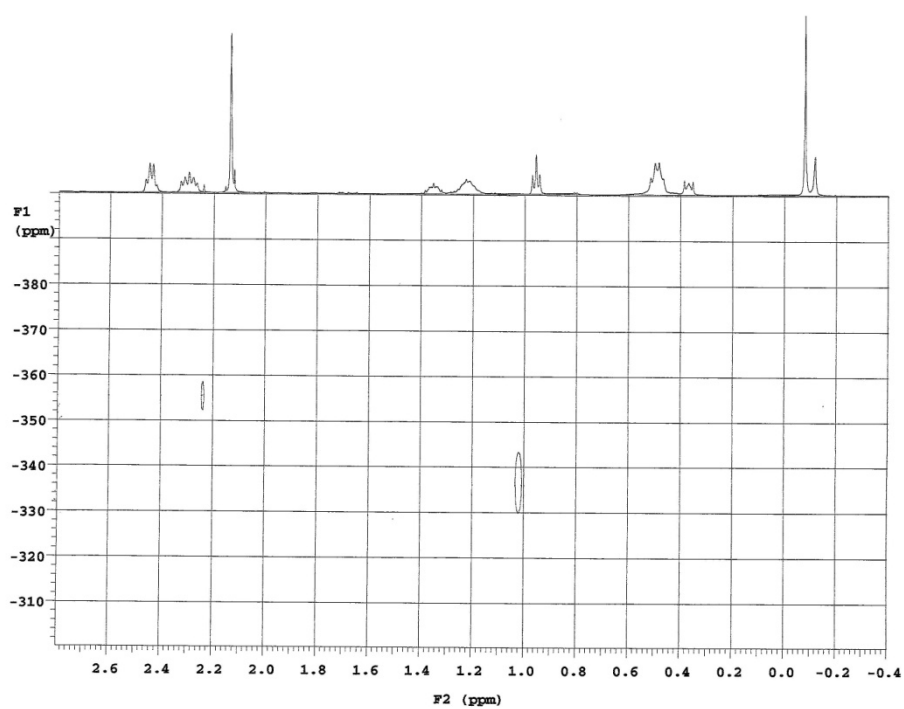


Figure S19. HMBC $\{^1\text{H}-^{15}\text{N}\}$ spectrum of $\text{G}_3\text{-}[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}_2)]_{16}$ (**5**) in CDCl_3 .

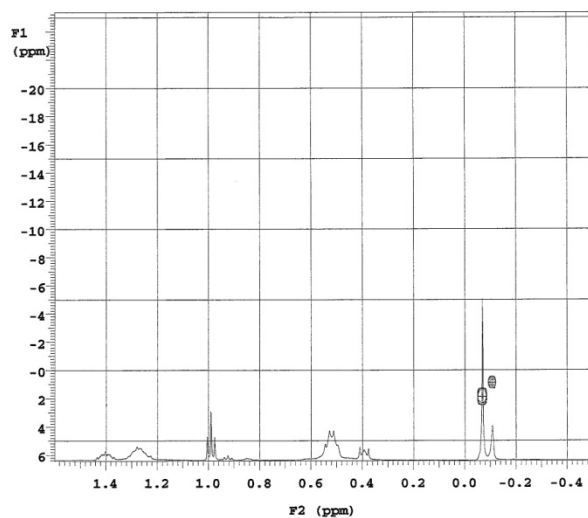


Figure S20. HMBC $\{^1\text{H}-^{29}\text{Si}\}$ spectrum of $\text{G}_3\text{-}[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}_2)]_{16}$ (**5**) in CDCl_3 .

F) $\{[\text{Et}_3\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+\text{H}(\text{Et})(\text{CH}_2\text{CH}_2\text{N}^+\text{HMe}_2)]_2\text{Cl}\}$ (6**)**

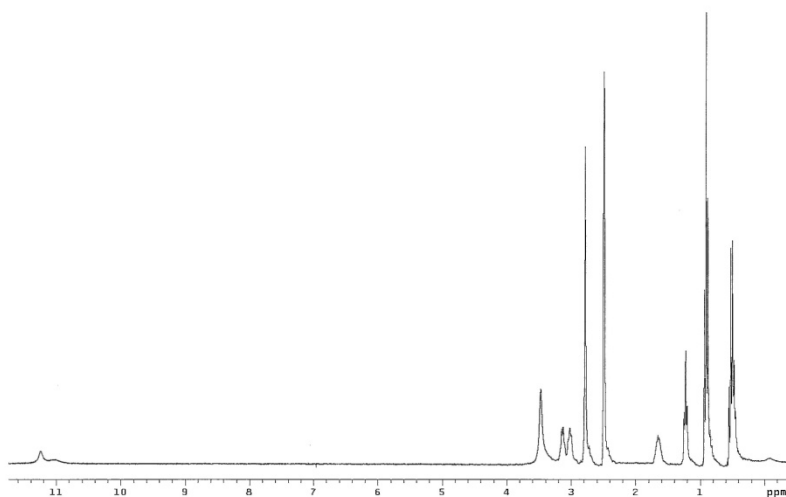


Figure S21. ^1H NMR spectrum of $\{[\text{Et}_3\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+\text{H}(\text{Et})(\text{CH}_2\text{CH}_2\text{N}^+\text{HMe}_2)]_2\text{Cl}\}$ (**6**) in DMSO .

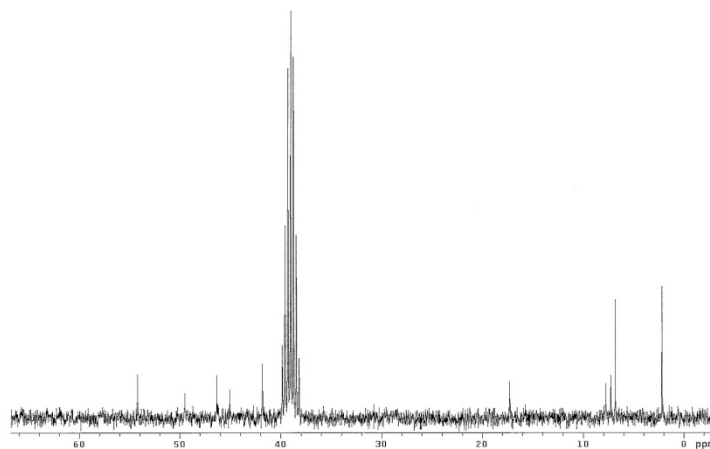


Figure S22. ^{13}C NMR spectrum of $\{[\text{Et}_3\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+\text{H}(\text{Et})(\text{CH}_2\text{CH}_2\text{N}^+\text{HMe}_2)]_2\text{Cl}^-\}$ (**6**) in DMSO.

G) $\text{G}_1\text{-}\{[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+\text{H}(\text{Et})(\text{CH}_2\text{CH}_2\text{N}^+\text{HMe}_2)]_4\text{8Cl}^-\}$ (7**)**

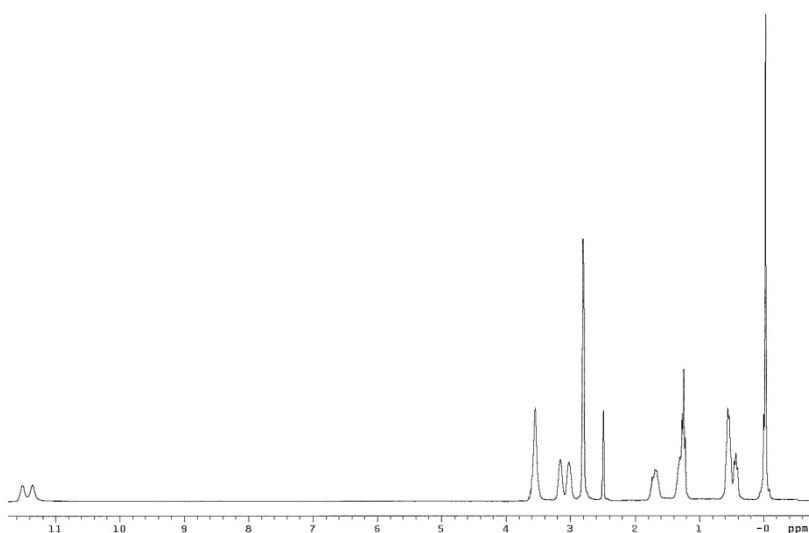


Figure S23. ^1H NMR spectrum of $\text{G}_1\text{-}\{[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+\text{H}(\text{Et})(\text{CH}_2\text{CH}_2\text{N}^+\text{HMe}_2)]_4\text{8Cl}^-\}$ (**7**) in DMSO.

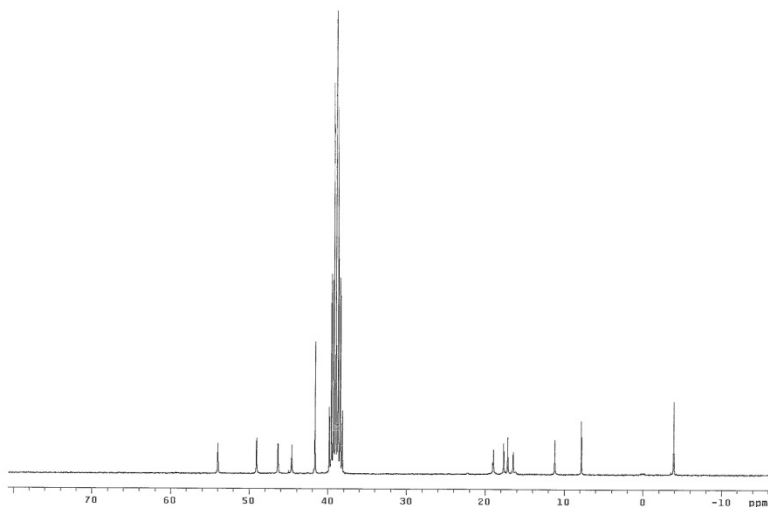


Figure S24. ^{13}C NMR spectrum of $\text{G}_1\text{-}\{[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2\text{N}^+\text{H}(\text{Et})(\text{CH}_2\text{CH}_2\text{N}^+\text{HMe}_2)]_4\text{8Cl}^-\}$ (**7**) in DMSO.

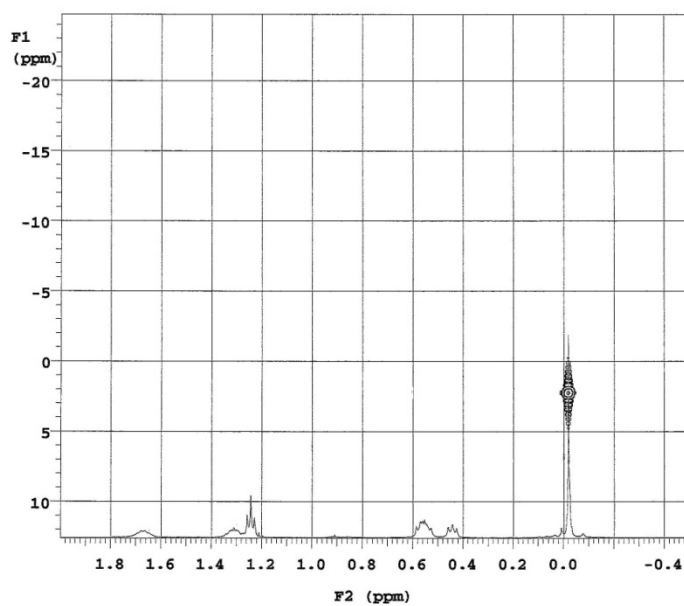


Figure S25. HMBC $\{^1\text{H}\text{-}^{29}\text{Si}\}$ spectrum of $\text{G}_1\text{-}\{[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2\text{N}^+\text{H}(\text{Et})(\text{CH}_2\text{CH}_2\text{N}^+\text{HMe}_2)]_4\text{8Cl}^-\}$ (**7**) in DMSO.

H) $G_2\text{-}\{[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+\text{H}(\text{Et})(\text{CH}_2\text{CH}_2\text{N}^+\text{HMe}_2)]_8\text{16Cl}\}$ (**8**)

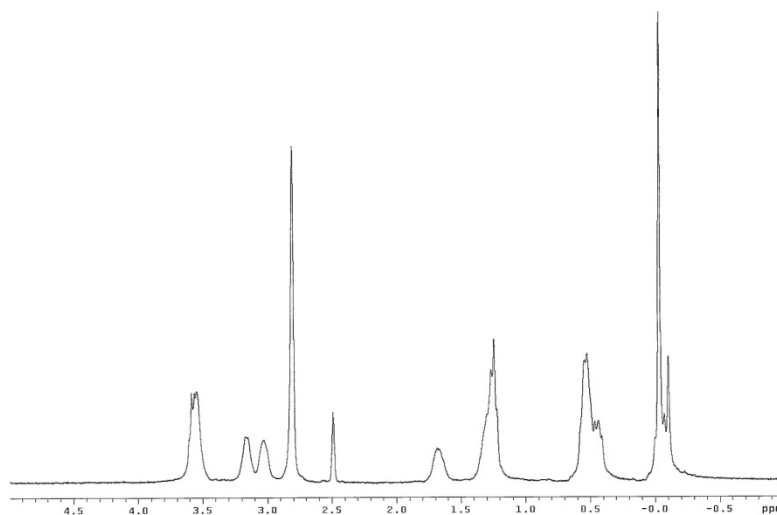


Figure S26. ^1H NMR spectrum of $G_2\text{-}\{[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+\text{H}(\text{Et})(\text{CH}_2\text{CH}_2\text{N}^+\text{HMe}_2)]_8\text{16Cl}\}$ (**8**) in DMSO.

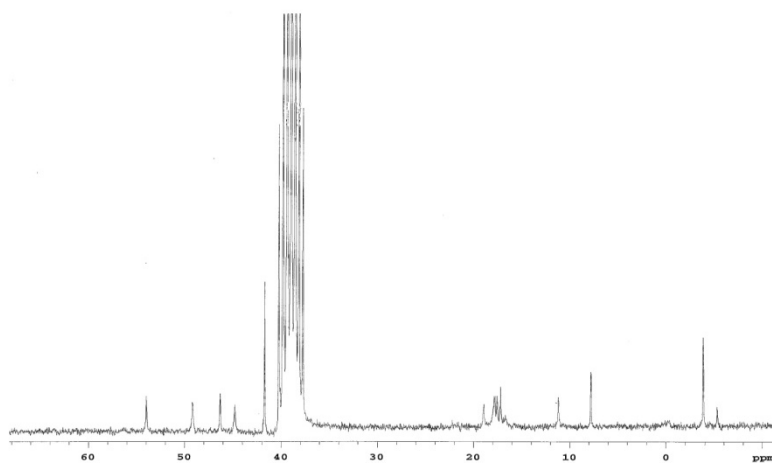


Figure S27. ^{13}C NMR spectrum of $G_2\text{-}\{[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+\text{H}(\text{Et})(\text{CH}_2\text{CH}_2\text{N}^+\text{HMe}_2)]_8\text{16Cl}\}$ (**8**) in DMSO.

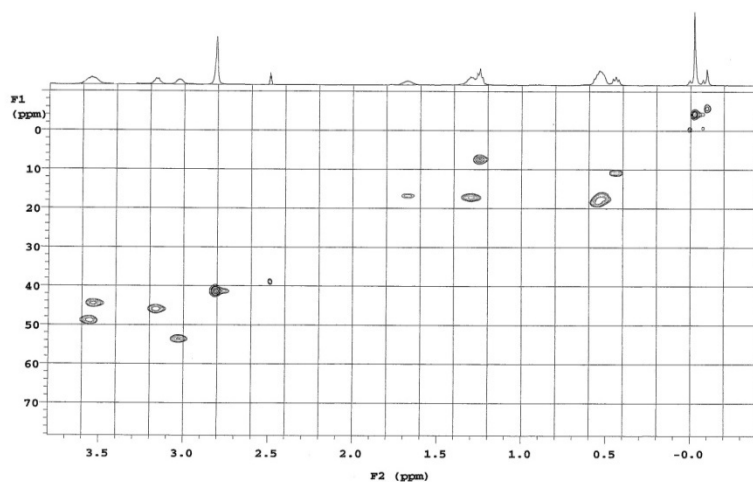


Figure S28. HMQC- $\{^1\text{H}-^{13}\text{C}\}$ spectrum of $\text{G}_2\text{-}\{[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+\text{H}(\text{Et})(\text{CH}_2\text{CH}_2\text{N}^+\text{HMe}_2)]_8\text{16Cl}\}$ (**8**) in DMSO.

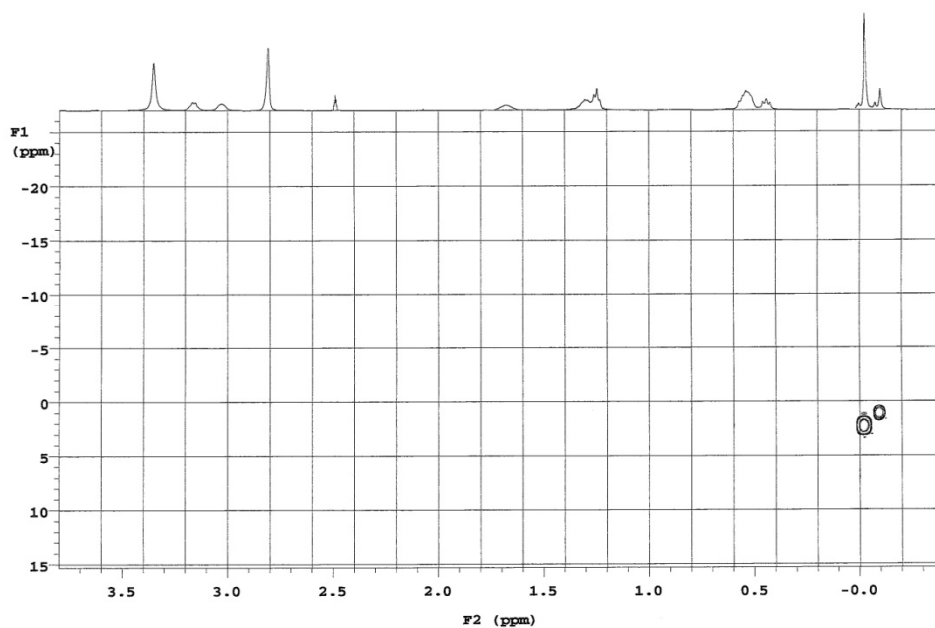


Figure S29. HMBC $\{^1\text{H}-^{29}\text{Si}\}$ spectrum of $\text{G}_2\text{-}\{[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+\text{H}(\text{Et})(\text{CH}_2\text{CH}_2\text{N}^+\text{HMe}_2)]_8\text{16Cl}\}$ (**8**) in DMSO.

I) $G_3\text{-}\{[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+\text{H}(\text{Et})(\text{CH}_2\text{CH}_2\text{N}^+\text{HMe}_2)]_{16}\text{32Cl}\}$ (9)

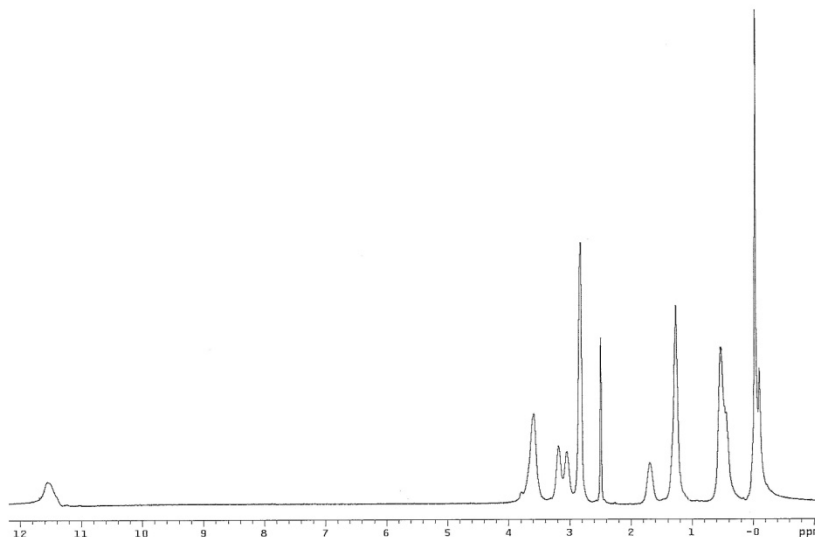


Figure S30. ^1H spectrum of $G_3\text{-}\{[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+\text{H}(\text{Et})(\text{CH}_2\text{CH}_2\text{N}^+\text{HMe}_2)]_{16}\text{32Cl}\}$ (9) in DMSO.

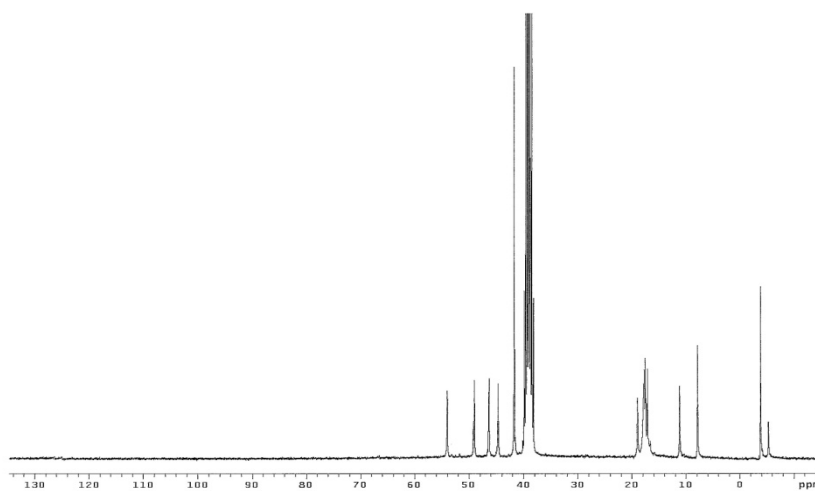


Figure S31. ^{13}C spectrum of $G_3\text{-}\{[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+\text{H}(\text{Et})(\text{CH}_2\text{CH}_2\text{N}^+\text{HMe}_2)]_{16}\text{32Cl}\}$ (9) in DMSO.

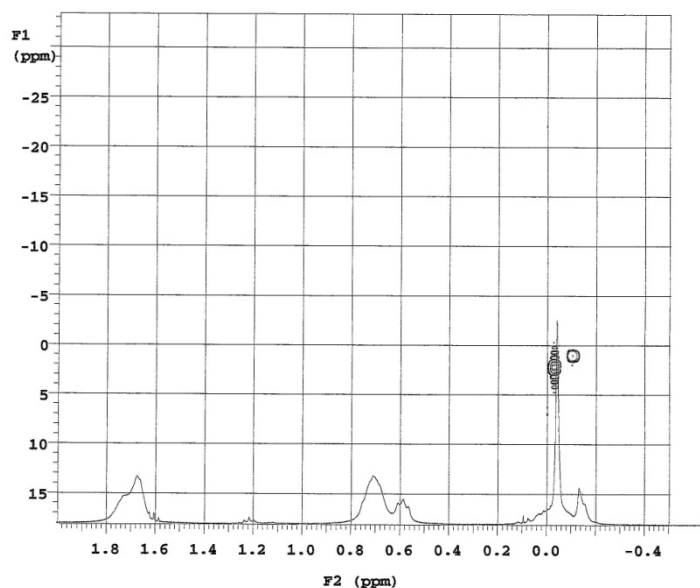


Figure S32. HMBC $\{^1\text{H}-^{29}\text{Si}\}$ spectrum of $\text{G}_3\text{-}\{[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+\text{H}(\text{Et})(\text{CH}_2\text{CH}_2\text{N}^+\text{HMe}_2)]_{16} \text{32Cl}^-\}$ (**9**) in DMSO.

J) $\{[\text{Et}_3\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+\text{Me}(\text{Et})(\text{CH}_2\text{CH}_2\text{N}^+\text{Me}_3)] \text{2I}^-\}$ (**10**)

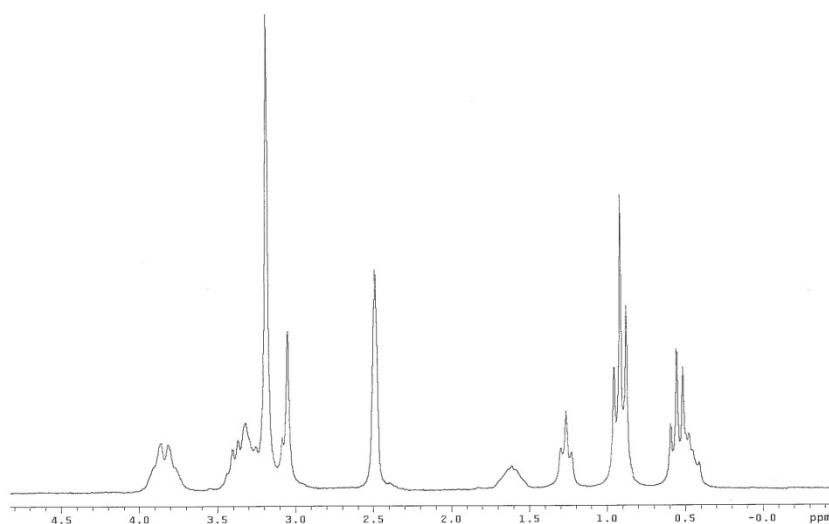


Figure S33. ^1H spectrum of $\{[\text{Et}_3\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+\text{Me}(\text{Et})(\text{CH}_2\text{CH}_2\text{N}^+\text{Me}_3)] \text{2I}^-\}$ (**10**) in DMSO.

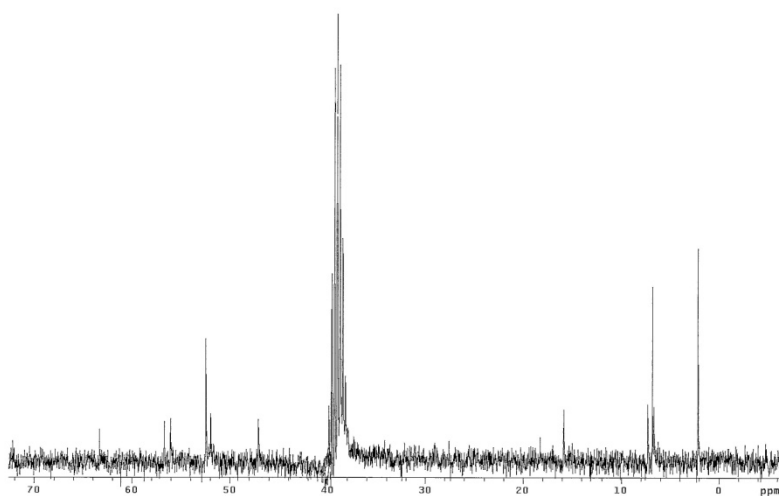


Figure S34. ^{13}C spectrum of $\{[\text{Et}_3\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+\text{Me}(\text{Et})(\text{CH}_2\text{CH}_2\text{N}^+\text{Me}_3)] 2\text{I}^-\}$ (**10**) in DMSO.

K) $\text{G}_1\text{-}\{\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+(\text{Me})(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}_3^+)\}_4 8\text{I}^-\}$ (**11**)

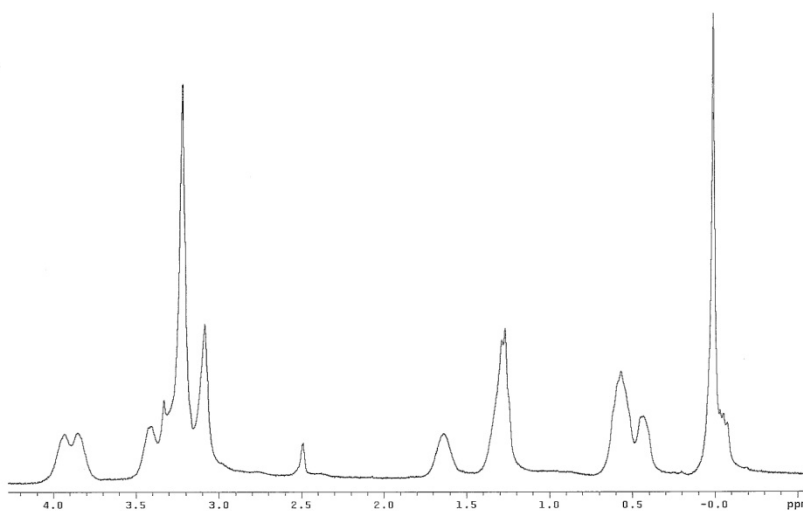


Figure S35. ^1H spectrum of $\text{G}_1\text{-}\{\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+(\text{Me})(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}_3^+)\}_4 8\text{I}^-\}$ (**11**) in DMSO.

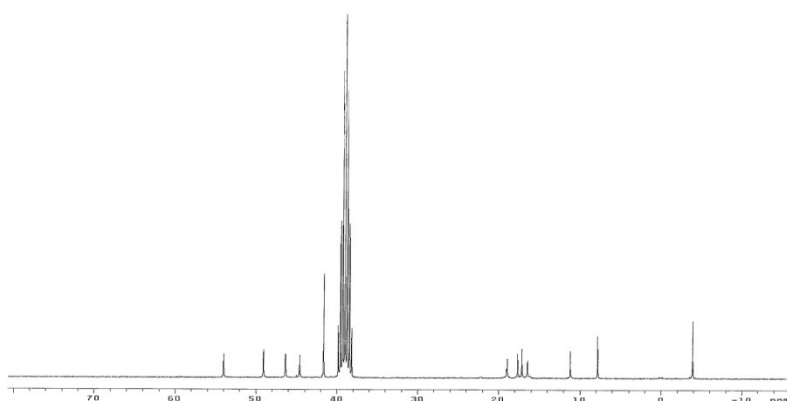


Figure S36. ^{13}C spectrum of $\text{G}_1\text{-}\{[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+(\text{Me})(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}^+_3)]_4\text{8I}^-\}$ (**11**) in DMSO.

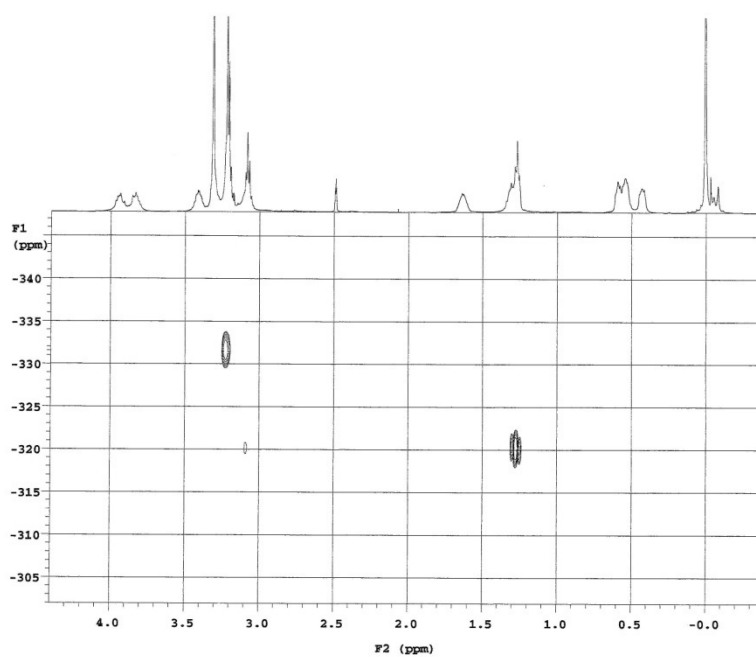


Figure S37. HMBC $\{^1\text{H}\text{-}^{15}\text{N}\}$ of $\text{G}_1\text{-}\{[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+(\text{Me})(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}^+_3)]_4\text{8I}^-\}$ (**11**) in DMSO.

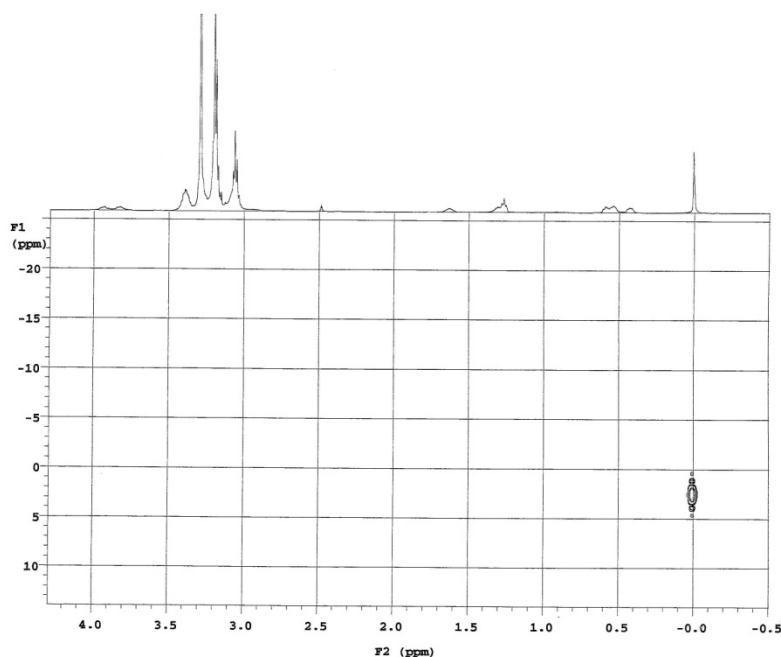


Figure S38. HMBC $\{^1\text{H}-^{29}\text{Si}\}$ spectrum of $\text{G}_1\text{-}\{\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+(\text{Me})(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}^+_3)_4\text{ 8I}^-\}$ (**11**) in DMSO.

L) $\text{G}_2\text{-}\{\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+(\text{Me})(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}^+_3)_8\text{ 16I}^-\}$ (**12**)

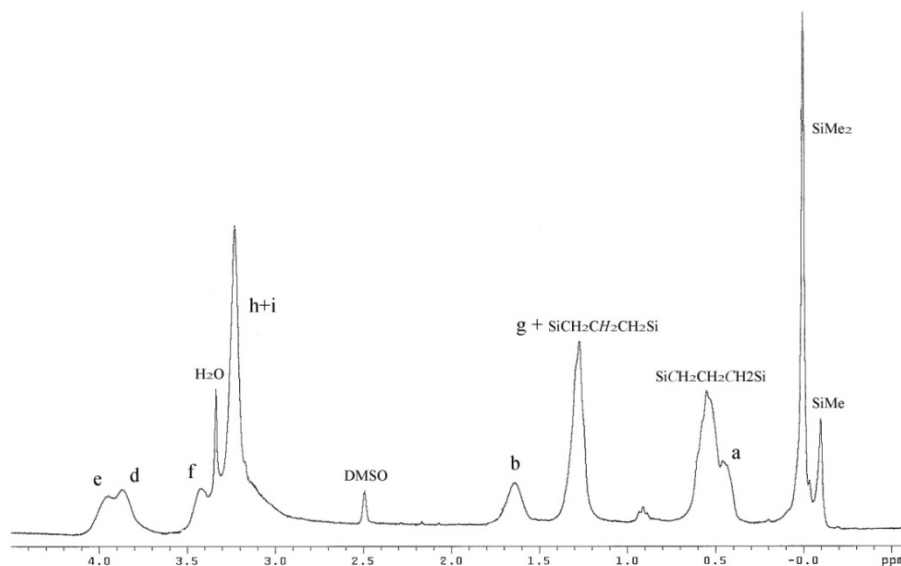


Figure S39. ^1H NMR spectrum of $\text{G}_2\text{-}\{\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+(\text{Me})(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}^+_3)_4\text{ 16I}^-\}$ (**12**) in DMSO.

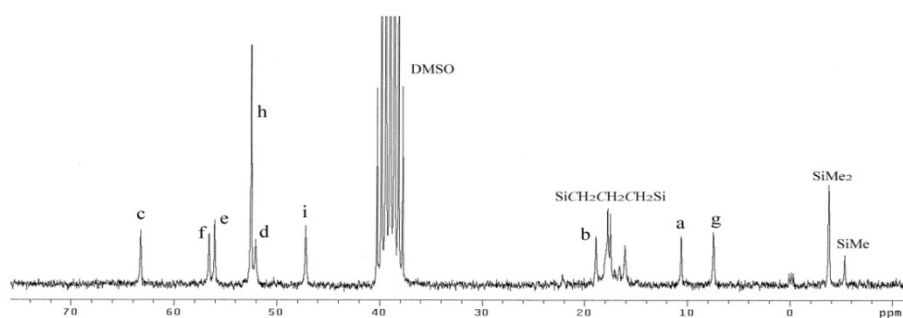


Figure S40. ^{13}C NMR spectrum of $\text{G}_2\text{-}\{[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+(\text{Me})(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}_3)_4\text{16I}^-\}$ (**12**) in DMSO.

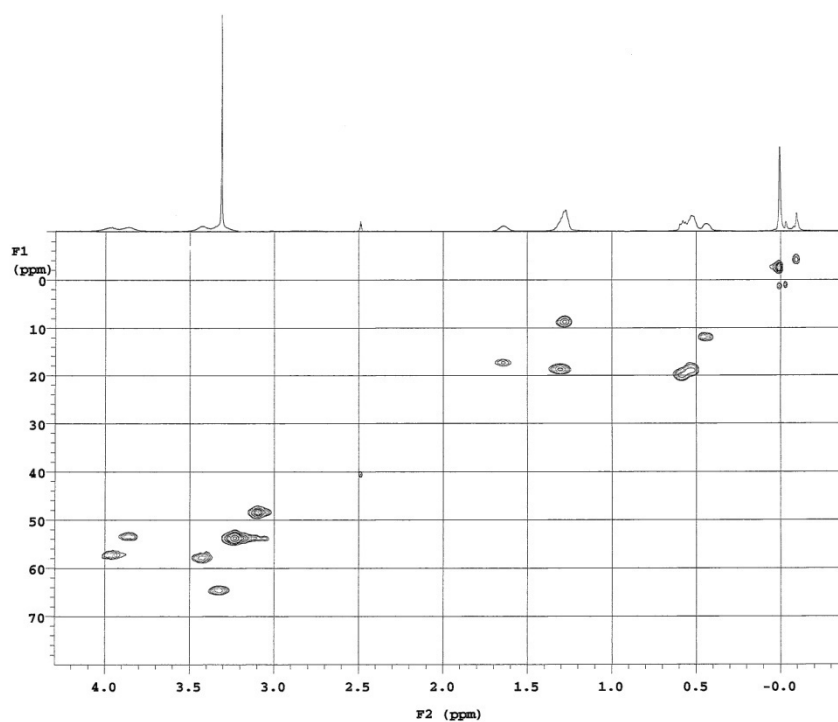


Figure S41. HMQC- $\{^1\text{H}\text{-}^{13}\text{C}\}$ spectrum of $\text{G}_2\text{-}\{[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+(\text{Me})(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}_3)_4\text{16I}^-\}$ (**12**) in DMSO.

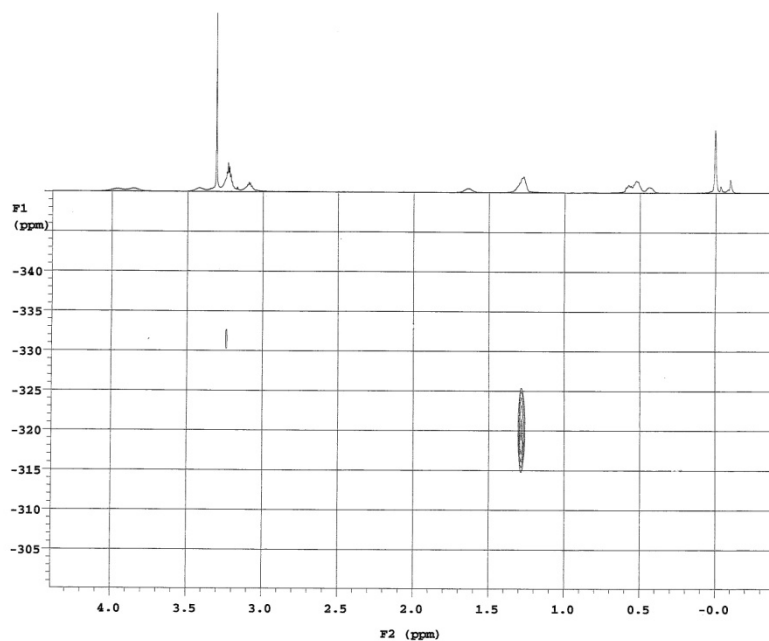


Figure S42. HMBC $\{^1\text{H}-^{15}\text{N}\}$ spectrum of $\text{G}_2\text{-}\{[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+(\text{Me})(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}_3)]_4\text{16I}^-\}$ (**12**) in DMSO.

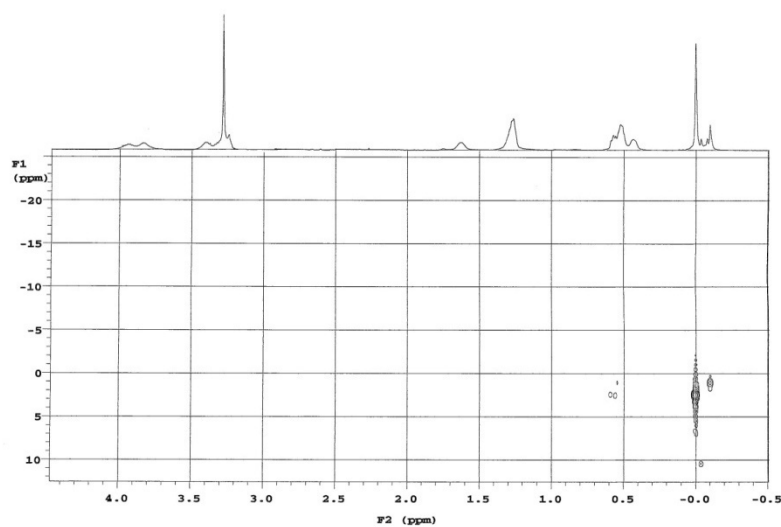


Figure S43. HMBC $\{^1\text{H}-^{29}\text{Si}\}$ spectrum of $\text{G}_2\text{-}\{[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+(\text{Me})(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}_3)]_4\text{16I}^-\}$ (**12**) in DMSO.

M) $G_3\text{-}\{\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+(\text{Me})(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}_3)\}_{16} 32\Gamma\}$ (13)

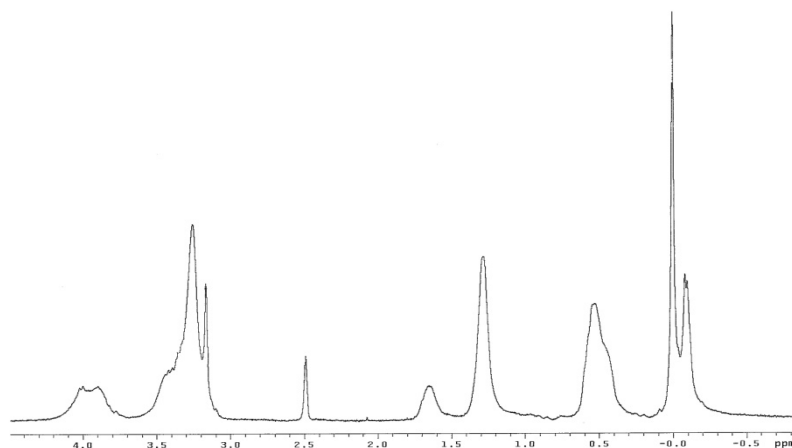


Figure S44. ^1H NMR spectrum of $G_3\text{-}\{\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+(\text{Me})(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}_3)\}_{16} 32\Gamma\}$ (13) in DMSO.

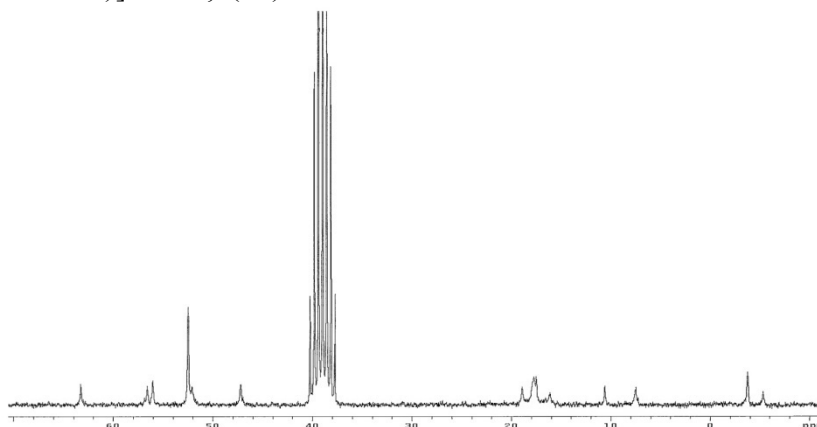


Figure S45. ^{13}C spectrum of $G_3\text{-}\{\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+(\text{Me})(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}_3)\}_{16} 32\Gamma\}$ (13) in DMSO.

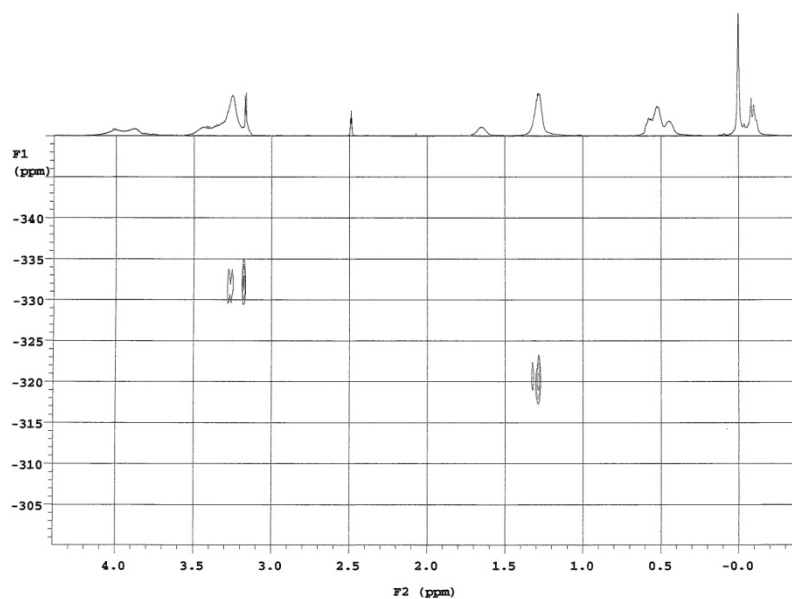


Figure S46. HMBC $\{^1\text{H}-^{15}\text{N}\}$ spectrum of $\text{G}_3\text{-}\{[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+(\text{Me})(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}_3)]_{16}\text{32}\Gamma\}$ (**13**) in DMSO.

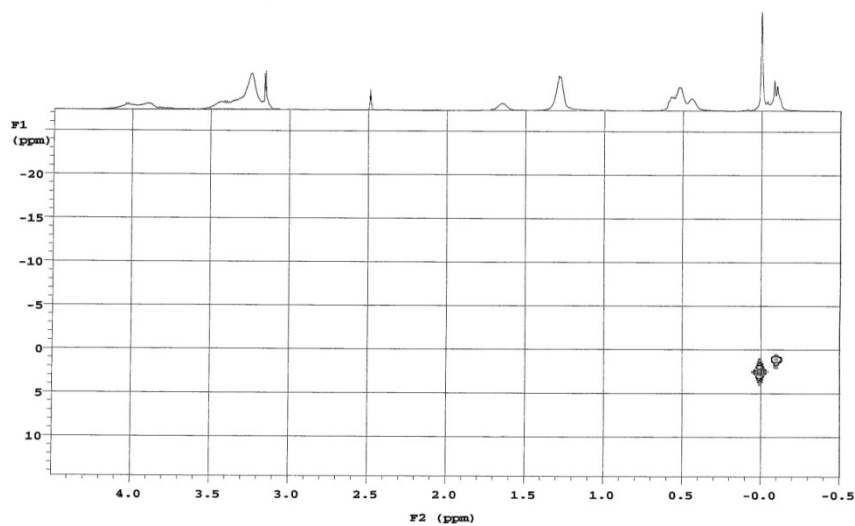


Figure S47. HMBC $\{^1\text{H}-^{29}\text{Si}\}$ spectrum of $\text{G}_3\text{-}\{[\text{Si}(\text{CH}_2\text{CH}_2\text{CH}_2)\text{N}^+(\text{Me})(\text{Et})(\text{CH}_2\text{CH}_2\text{NMe}_3)]_{16}\text{32}\Gamma\}$ (**13**) in DMSO.